A MATHEMATICAL ANALYSIS OF THE LEAST SQUARES SENSITIVITY METHOD

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Abstract. For a parameterized hyperbolic system $u_{i+1} = f(u_i, s)$, the derivative of an ergodic average $\langle J \rangle = \lim_{n\to\infty} \frac{1}{n}\sum_1^n J(u_i, s)$ to the parameter s can be computed via the least squares sensitivity method. This method solves a constrained least squares problem and computes an approximation to the desired derivative $\frac{d\langle J\rangle}{ds}$ from the solution. This paper proves that as the size of the least squares problem approaches infinity, the computed approximation converges to the true derivative.

Key words. Sensitivity analysis, linear response, least squares sensitivity, hyperbolic attractor, chaos, statistical average, ergodicity

AMS subject classifications.

1. Introduction.

Consider a family of C^1 bijection maps $f(u, s) : \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}^m$ parameterized by $s \in \mathbb{R}$. We are also given a C^1 function $J(u, s) : \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}$. We assume that the system is *ergodic*, i.e., the infinite time average

$$\langle J \rangle = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} J(u_i, s)\ , \quad \text{where} \quad u_{i+1} = f(u_i, s),\ i = 1, \dots \tag{1.1}$$

depends on s but does not depend on the initial state u_0. The *least squares sensitivity* method attempts to compute its derivative via

Theorem LSS. *Under ergodicity and hyperbolicity assumptions (details in Section 6),*

$$\frac{d\langle J\rangle}{ds} = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} (DJ(u_i, s))\, v_i^{\{n\}} + (\partial_s J(u_i, s))\ , \tag{1.2}$$

where $v_i^{\{n\}} \in \mathbb{R}^m, i = 1, \dots, n$ *is the solution to the constrained least squares problem*

$$\min \frac{1}{2} \sum_{i=1}^{n} v_i^{\{n\}T} v_i^{\{n\}} \quad s.t. \quad v_{i+1}^{\{n\}} = (Df(u_i, s))\, v_i^{\{n\}} + (\partial_s f(u_i, s))\ , \tag{1.3}$$

$i = 1, \dots, n-1$. Here the linearized operators are defined as

$$\begin{aligned}
(DJ(u, s))\, v &:= (D_v J)(u, s) := \lim_{\epsilon\to 0} \frac{J(u + \epsilon v, s) - J(u, s)}{\epsilon} \\
(Df(u, s))\, v &:= (D_v f)(u, s) := \lim_{\epsilon\to 0} \frac{f(u + \epsilon v, s) - f(u, s)}{\epsilon} \\
(\partial_s J(u, s)) &:= \lim_{\epsilon\to 0} \frac{J(u, s + \epsilon) - J(u, s)}{\epsilon} \\
(\partial_s f(u, s)) &:= \lim_{\epsilon\to 0} \frac{f(u, s + \epsilon) - f(u, s)}{\epsilon}
\end{aligned} \tag{1.4}$$

$(DJ), (\partial_s J), (Df)$ and $(\partial_s f)$ are a $1 \times m$ matrix, a scalar, an $m \times m$ matrix and an $m \times 1$ matrix, respectively, representing the partial derivatives.

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Computation of the derivative $d\langle J\rangle/ds$ represents a class of important problems in computational science and engineering. Many applications involve simulation of nonlinear dynamical systems that exhibit chaos. Examples include weather and climate, turbulent combustion, nuclear reactor physics, plasma dynamics in fusion, and multi-body problems in molecular dynamics. The quantities that are to be predicted (the so-called quantities of interest) are often time averages or expected values $\langle J\rangle$. Derivatives of these quantities of interests to parameters are required in applications including

- **Numerical optimization**. The derivative of the objective function $\langle J\rangle$ with respect to the design, parameterized by s, is used by gradient-based algorithm to efficiently optimize in high dimensional design spaces.
- **Uncertainty quantification**. The derivative of the quantities $\langle J\rangle$ with respect to the sources of uncertainties s can be used to assess the error and uncertainty in the computed $\langle J\rangle$.

Traditional transient sensitivity analysis methods fail to compute $d\langle J\rangle/ds$ in chaotic systems. These methods focus on linearizing initial value problems to obtain the derivative of the quantities of interest. When the quantity of interest is a long-time average in a chaotic system, the derivative of this average does not equal the long time average of the derivative. As a result, traditional adjoint methods fail, and the root of this failure is the ill-conditioning of initial value problems of chaotic systems [6].

The differentiability of $\langle J\rangle$ has been shown by Ruelle [8]. Ruelle also constructed a formula of the derivative. However, Ruelle's formula is difficult to compute numerically [6, 4]. Abramov and Majda are successful in computing the derivative based on the fluctuation dissipation theorem [1]. However, for systems whose SRB measure [13] deviates strongly from Gaussian, fluctuation dissipation theorem based methods can be inaccurate. Several more recent methods have been developed for computing this derivative [10, 11, 2, 12]. In particular, the *least squares sensitivity* method [12] is a simple method that computes the derivative of $\langle J\rangle$ efficiently.

This paper provides theoretical foundation for the least squares sensitivity method by proving Theorem (LSS) for uniformly hyperbolic maps. Section 2 lays out the basic assumptions, and introduces hyperbolicity for readers who are not familiar with this concept. Section 3 then proves a special version of the classic structural stability result, and defines the shadowing direction, a key concept used in our proof. Section 4 demonstrates that the derivative of $\langle J\rangle$ can be computed through the shadowing direction. Section 5 then shows that the least squares sensitivity method is an approximation of the shadowing direction. Section 6 finally proves Theorem LSS by showing that the approximation of the shadowing direction makes a vanishing error in the computed derivative of $\langle J\rangle$.

2. Uniform hyperbolicity. This section consider a dynamical system governed by

$$u_{i+1} = f(u_i, s) \tag{2.1}$$

with a parameter $s \in \mathbb{R}$, where $u_i \in \mathbb{R}^m$ and $f : \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}^m$ is C^1 and bijective in u. This paper studies perturbation of s around a nominal value. Without loss of generality, we assume the nominal value of s to be 0. We denote $f^{(0)}(u, s) \equiv u$ and $f^{(i+1)}(u, s) \equiv f^{(i)}(f(u, s), s)$ for all $i \in \mathbb{Z}$.

We assume that the map has a *compact, global, uniformly hyperbolic attractor* $\Lambda \subset \mathbb{R}^m$ at $s = 0$, satisfying

1. For all $u_0 \in \mathbb{R}^m$, $dist(\Lambda, f^{(n)}(u_0,0)) \xrightarrow{n\to\infty} 0$ where $dist$ is the Euclidean distance in $\mathbb{R}^m$.
2. There is a $C \in (0,\infty)$ and $\lambda \in (0,1)$, such that for all $u \in \Lambda$, there is a splitting of $\mathbb{R}^m$ representing the space of perturbations around u.

$$\mathbb{R}^m = V^+(u) \oplus V^-(u) \;, \tag{2.2}$$

where the subspaces are
   - $V^+(u) := \{v \in \mathbb{R}^m : \|(Df^{(i)}(u,0))\, v\| \le C\,\lambda^{-i}\,\|v\| \;, \forall i < 0\}$ is the *unstable subspace* at u, where $\|\cdot\|$ is the Euclidean norm in $\mathbb{R}^m$, and

$$\begin{aligned}(Df^{(i)}(u,s))\, v :=& \lim_{\epsilon\to 0} \frac{f^{(i)}(u+\epsilon v, s) - f^{(i)}(u,s)}{\epsilon} \\ =&(Df^{(i-1)}(f(u,s),s))\;(Df(u,s))\;v\end{aligned}$$

   - $V^-(u) := \{v \in \mathbb{R}^m : \|(Df^{(i)}(u,0))\, v\| \le C\,\lambda^{i}\,\|v\| \;, \forall i > 0\}$ is the *stable subspace* at u.

   Both $V^+(u)$ and $V^-(u)$ are continuous with respect to u.

It can be shown that the subspaces $V^+(u)$ and $V^-(u)$ are *invariant* under the differential of the map (Df), i.e., if $u' = f(u,0)$ and $v' = (Df(u,0))\, v$, then [9]

$$v \in V_s^+(u) \Longleftrightarrow v' \in V_s^+(u') \;, \quad v \in V_s^-(u) \Longleftrightarrow v' \in V_s^-(u') \;. \tag{2.3}$$

Uniformly hyperbolic chaotic dynamical systems are known as "ideal chaos". Because of its relative simplicity, studies of hyperbolic chaos has generated enormous insight into the properties of chaotic dynamical systems [5]. Although most dynamical systems encountered in science and engineering are not uniformly hyperbolic, many of them are classified as *quasi-hyperbolic*. These systems, including the famous Lorenz system, have global properties similar to those of uniformly hyperbolic systems [3]. Results obtained on uniformly hyperbolic systems can often be generalized to quasi-hyperbolic ones. Scholars believe that very complex dynamical systems like turbulence are quasi-hyperbolic []. Although this paper focuses on proving the convergence of the least squares sensitivity method for uniformly hyperbolic systems, is has been shown numerically that this method also works when the system is not uniformly hyperbolic [12].

3. Structural stability and the shadowing direction. The hyperbolic structure (2.2) ensures the *structurally stability* of the attractor Λ under perturbation in s. Here we prove a specialized version of the structural stability result.

THEOREM 1. *If (2.2) holds and f is continuously differentiable, then for all sequence $\{u_i^0, i \in \mathbb{Z}\} \subset \Lambda$ satisfying $u_{i+1}^0 = f(u_i^0, 0)$, there is a $\delta > 0$ such that for all $|s| < \delta$ there is a unique sequence $\{u_i^s, i \in \mathbb{Z}\} \subset \mathbb{R}^m$ satisfying $\|u_i^s - u_i^0\| < \delta$ and $u_{i+1}^s = f(u_i^s, s)$ for all $i \in \mathbb{Z}$. Furthermore, u_i^s is i-uniformly continuously differentiable to s.*

Note: i-uniformly continuous differentiability of u_i^s means $\forall s \in (-\delta,\delta)$ and $\epsilon > 0 : \exists \delta : |s'-s| < \delta \Rightarrow \left\| \frac{du_i^s}{ds}\Big|_s - \frac{du_i^s}{ds}\Big|_{s'} \right\| < \epsilon$ for all i. Other than the i-uniformly continuous differentiability of u_i^s, this theorem can be obtained directly from the shadowing lemma[7]. However, the uniformly continuous differentiability result requires a more in-depth proof. A more general version of this result has been proved by Ruelle[8].

To prove the theorem, we denote $\mathbf{u} = \{u_i, i \in \mathbb{Z}\}$. The norm

$$\|\mathbf{u}\|_{\mathcal{B}} = \sup_{i\in\mathbb{Z}} \|u_i\| \tag{3.1}$$

defines a Banach space $\mathcal{B}$ of uniformly bounded sequences in $\mathbb{R}^m$. Define the map $F : \mathcal{B} \times \mathbb{R} \to \mathcal{B}$ as $F(\mathbf{u}, s) = \{u_i - f(u_{i-1}, s),\ i \in \mathbb{Z}\}$. We use the implicit function theorem to complete the proof, which requires F to be differentiable and its derivative to be non-singular at $\mathbf{u}^0$.

Lemma 2. *Under the conditions of Theorem 1, F has Fréchet derivative at all $\mathbf{u} \in \mathcal{B}$:*

$$(DF(\mathbf{u}, s))\,\mathbf{v} = \{v_i - (Df(u_{i-1}, s))\,v_{i-1}\}\ , \quad \textit{where} \quad \mathbf{v} = \{v_i\}$$

Proof. Because $\|\mathbf{u}\|_{\mathcal{B}} = \sup_i \|u_i\| < \infty$, we can find $C > 2\|u_i\|$ for all i. Because $f \in C^1$, its derivative (Df) is uniformly continuous in the compact set $\{u : \|u\| \le C\}$. For $\|\mathbf{v}\|_{\mathcal{B}} < C/2$, we apply the mean value theorem to obtain

$$\frac{f(u_i + v_i, s) - f(u_i, s)}{\|\mathbf{v}\|_{\mathcal{B}}} - \frac{(Df(u_i, s))\,v_i}{\|\mathbf{v}\|_{\mathcal{B}}} = \frac{(Df(u_i + \xi v_i, s)) - (Df(u_i, s))}{\|\mathbf{v}\|_{\mathcal{B}}}\,v_i$$

where $0 \le \xi \le 1$. Because $\|u_i + \xi v_i\| \le \|u_i\| + \|v_i\| < C$ for all i, uniform continuity of (Df) implies that $\forall\epsilon > 0, \exists\delta$ such that for all $\sup\|v_i\| < \delta$,

$$\left\|\frac{(Df(u_i + \xi v_i, s)) - (Df(u_i, s))}{\|\mathbf{v}\|_{\mathcal{B}}}\,v_i\right\| \le \|Df(u_i + \xi v_i, s)) - (Df(u_i, s)\| < \epsilon$$

for all i. Therefore,

$$\begin{aligned}\frac{F(\mathbf{u}+\mathbf{v}, s) - F(\mathbf{u}, s)}{\|\mathbf{v}\|_{\mathcal{B}}} &= \left\{\frac{v_i}{\|\mathbf{v}\|_{\mathcal{B}}} - \frac{f(u_{i-1} + v_{i-1}, s) - f(u_{i-1}, s)}{\|\mathbf{v}\|_{\mathcal{B}}}\right\} \\ &\longrightarrow \frac{\{v_i - (Df(u_{i-1}, s))\,v_{i-1}\}}{\|\mathbf{v}\|_{\mathcal{B}}}\end{aligned}$$

in the $\mathcal{B}$ norm. Now we only need to show that the linear map $\{v_i\} \to \{v_i - (Df(u_{i-1}, s))\,v_{i-1}\}$ is bounded. This is because (Df) is continuous, thus it is uniformly bounded in the compact set $\{u : \|u\| \le C\}$. Denote the bound in this compact set as $\|(Df)\| < A$, then $\left\|\{v_i - (Df(u_{i-1}, s))\,v_{i-1}\}\right\|_{\mathcal{B}} \le (1 + A)\ \|\{v_i\}\|_{\mathcal{B}}$. ∎

Lemma 3. *Under conditions of Theorem 1, the Fréchet derivative of F at $\mathbf{u}^0$ and $s = 0$ is a bijection.*

Proof. The Fréchet derivative of F at $\mathbf{u}^0$ and $s = 0$ is

$$(DF(\mathbf{u}^0, 0))\,\mathbf{v} = \{v_i - (Df(u^0_{i-1}, 0))\,v_{i-1}\}$$

We only need to show that for every $\mathbf{r} = \{r_i\} \in \mathcal{B}$, there exists a unique $\mathbf{v} = \{v_i\} \in \mathcal{B}$ such that $v_i - (Df(u^0_{i-1}, 0))\,v_{i-1} = r_i$ for all i.

Because of (2.2), we can first split $r_i = r_i^+ + r_i^-$, where $r_i^+ \in V^+(u_i)$ and $r_i^- \in V^-(u_i)$. Because $V^+(u)$ and $V^-(u)$ are continuous to u and Λ is compact,

$$\inf_{\substack{u\in\Lambda \\ r^\pm \in V^\pm(u)}} \frac{\|r^+ + r^-\|}{\max(\|r^+\|, \|r^-\|)} = \beta > 0\ .$$

(This is because if $\beta = 0$, then by the continuity of $V^+(u), V^-(u)$ and the compactness of $\big\{(u, r^+, r^-) \in \Lambda \times \mathbb{R}^m \times \mathbb{R}^m : \max(\|r^+\|, \|r^-\|) = 1\big\}$, there must be a $u \in \Lambda, r^+ \in V^+(u), r^- \in V^-(u)$ such that $\max(\|r^+\|, \|r^-\|) = 1$ and $r^+ + r^- = 0$, which contradicts to the hyperbolicity assumption (2.2)). Therefore,

$$\max(\|r_i^+\|, \|r_i^-\|) \le \frac{\|r_i\|}{\beta} \le \frac{\|\mathbf{r}\|_{\mathcal{B}}}{\beta} \quad \text{for all } i$$

Now let

$$v_i = \sum_{j=0}^{\infty} (Df^{(j)}(u_i)\, r_{i-j}^- - \sum_{j=1}^{\infty} (Df^{(-j)}(u_i)\, r_{i+j}^+ \ ,$$

It can be verified that $v_i - (Df(u_{i-1}^0, 0))\, v_{i-1} = r_i$, and by the definition of $V^+(u)$ and $V^-(u)$,

$$\begin{aligned} \|v_i\| &\le \sum_{j=0}^{\infty} \left\|(Df^{(j)})(u_i)\, r_{i-j}^-\right\| + \sum_{j=1}^{\infty} \left\|(Df^{(-j)})(u_i)\, r_{i+j}^+\right\| \\ &\le \sum_{j=0}^{\infty} C\,\lambda^j \|r_{i-j}^-\| + \sum_{j=1}^{\infty} C\,\lambda^j \|r_{i+j}^+\| \le \frac{2C}{1-\lambda} \frac{\|\mathbf{r}\|_{\mathcal{B}}}{\beta} \ , \end{aligned} \tag{3.2}$$

Therefore, v_i is uniformly bounded for all i. Thus $\mathbf{v} \in \mathcal{B}$.

Because of linearity, uniqueness of $\mathbf{v}$ such that $v_i - (Df(u_{i-1}^0, 0))\, v_{i-1} = r_i$ only need to be shown for $\mathbf{r} = \mathbf{0}$. To show this, we split $v_i = v_i^+ + v_i^-$ where $v_i^+ \in V^+(u_i)$ and $v_i^- \in V^-(u_i)$. Because the spaces $V^+(u_i)$ and $V^-(u_i)$ are invariant (Equation 2.3),

$$0 = r_i = \big(v_i^+ - (Df(u_{i-1}^0, 0))\, v_{i-1}^+\big) + \big(v_i^- - (Df(u_{i-1}^0, 0))\, v_{i-1}^-\big)$$

where the two parentheses are in $V^+(u_i)$ and $V^-(u_i)$, respectively. Because $V^+(u_i) \cap V^-(u_i) = \{0\}$, both parentheses in the equation above must be 0 for all i, and

$$\begin{aligned} v_i^+ &= (Df(u_{i-1}^0, 0))\, v_{i-1}^+ = \ldots = (Df^{(i-j)}(u_j^0, 0)\, v_j^+ \\ v_i^- &= (Df(u_{i-1}^0, 0))\, v_{i-1}^- = \ldots = (Df^{(i-j)}(u_j^0, 0)\, v_j^- \end{aligned} \quad \text{for all } i > j \ .$$

By the definition of $V^+(u_i)$ and $V^-(u_i)$, $\|v_j^+\| \le C\lambda^{i-j}\|v_i^+\|$, $\|v_i^-\| \le C\lambda^{i-j}\|v_j^-\|$. If $v_j^+ \ne 0$ for some j, then

$$\frac{\|v_i\|}{\beta} \ge \|v_i^+\| \ge \frac{\lambda^{j-i}}{C}\|v_j^+\| \quad \text{for all} \quad i > j \ ,$$

and $\{v_i, i \in \mathbb{Z}\}$ is unbounded. Similarly, if $v_i^- \ne 0$ for some i, then

$$\frac{\|v_j\|}{\beta} \ge \|v_j^-\| \ge \frac{\lambda^{j-i}}{C}\|v_i^-\| \quad \text{for all} \quad j < i \ ,$$

and $\{v_i, i \in \mathbb{Z}\}$ is unbounded. Therefore, for $\{v_i\}$ to be bounded, we must have $v_i = v_i^+ + v_i^- = 0$ for all i. This proves the uniqueness of $\mathbf{v}$ for $\mathbf{r} = \mathbf{0}$. ∎

Proof. [Proof of Theorem 1.] $F(\mathbf{u}^0, 0) = \{u_i^0 - f(u_{i-1}^0, 0)\} = \mathbf{0}$. So $\mathbf{u}^0$ is a zero point of F at $s = 0$. Combining this with the two lemma above enables application of

the implicit function theorem. Thus there exists $\delta > 0$ such that for all $|s| < \delta$ there is a unique $\mathbf{u}^s = \{u_i^s\}$ satisfying $\|\mathbf{u}^s - \mathbf{u}^0\|_{\mathcal{B}} < \delta$ and $F(\mathbf{u}^s, s) = 0$. Furthermore, $\mathbf{u}^s$ is continuously differentiable to s, i.e., $\frac{d\mathbf{u}^s}{ds} \in \mathcal{B}$ is continuous with respect to s in the $\mathcal{B}$ norm. By the definition of derivatives (in $\mathcal{B}$ and in $\mathbb{R}^m$), $\frac{d\mathbf{u}^s}{ds} = \left\{\frac{du_i^s}{ds}\right\}$. Continuity of $\frac{d\mathbf{u}^s}{ds}$ in $\mathcal{B}$ then implies that $\frac{du_i^s}{ds}$ is i-uniformly continuous with respect to s. ∎

Theorem 1 states that for a series $\{u_i^0\}$ satisfying the governing equation (2.1) at $s = 0$, there is a series $\{u_i^s\}$ satisfying the governing equation at nearby values of s. In addition, u_i^s *shadows* u_i^0, i.e., u_i^s is close to u_i^0 when s is close to 0. Also, $\left\{\frac{du_i^s}{ds}\Big|_{s=0}\right\}$ exists and is i-uniformly bounded.

Definition 4. *The* **shadowing direction** $v_i^{\{\infty\}}$ *is defined as the uniformly bounded series*

$$\mathbf{v}^{\{\infty\}} := \left\{v_i^{\{\infty\}}\right\} := \left\{\frac{du_i^s}{ds}\Big|_{s=0}\right\} = \frac{d\mathbf{u}^s}{ds}\Big|_{s=0} \in \mathcal{B}\,,$$

where u_i^s is defined by Theorem 1.

The shadowing direction is the direction in which the shadowing series u_i^s moves as s increases from 0. It provides a vehicle by which we prove Theorem LSS. We show that the derivative of the ergodic mean $\langle J\rangle$ to s can be obtained if the shadowing direction $v_i^{\{\infty\}}$ was given (Section 4). We then show that $v_i^{\{n\}}$, the solution to the constrained least squares problem (1.3), sufficiently approximates the shadowing direction $v_i^{\{\infty\}}$ when n is large (Section 5). We finaly show in Section 6) that the same derivative can be obtained from the least squares solution $v_i^{\{n\}}$.

4. Ergodic mean derivative via the shadowing direction. This section proves an easier version of Theorem LSS that replaces the solution to the constrained least squares problem $v_i^{\{n\}}, i = 1, \ldots, n$ by the shadowing direction $v_i^{\{\infty\}} = \frac{du_i^s}{ds}\big|_{s=0}$.

Theorem 5. *If (2.2) holds and f is continuously differentiable, For all continuously differentiable function $J(u, s) : \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}$ whose infinite time average*

$$\langle J\rangle := \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} J(f^{(i)}(u_0, s), s) \tag{4.1}$$

is independent of the initial state $u_0 \in \mathbb{R}^m$, let $\{v_i^{\{\infty\}}, i \in \mathbb{Z}\}$ be the sequence of shadowing direction in Definition 4, then

$$\frac{d\langle J\rangle}{ds}\bigg|_{s=0} = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \Big((DJ(u_i^0, 0))v_i^{\{\infty\}} + (\partial_s J(u_i^0, 0))\Big)\ , \tag{4.2}$$

Proof. This proof is essentially an exchange of limits through uniform convergence. Because $\langle J\rangle$ in Equation (4.1) independent of u_0, we set $u_0 = u_0^s$ in Theorem 1 (thus $f^{(i)}(u_0^s, s) = u_i^s$) and obtain

$$\frac{d\langle J\rangle}{ds}\bigg|_{s=0} = \lim_{s\to 0} \frac{\langle J\rangle|_{s=s} - \langle J\rangle|_{s=0}}{s} = \lim_{s\to 0}\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \frac{J(u_i^s, s) - J(u_i^0, 0)}{s}$$

Denote

$$\gamma_i^s = \frac{dJ(u_i^s, s)}{ds} = (DJ(u_i^s, s))\frac{du_i^s}{ds} + (\partial_s J(u_i^s, s))$$

and use the mean value theorem, we obtain

$$\left.\frac{d\langle J\rangle}{ds}\right|_{s=0} = \lim_{s\to 0}\lim_{n\to\infty}\frac{1}{n}\sum_{i=1}^{n}\gamma_i^{\xi_i(s)}\ ,\quad \text{where all } |\xi_i(s)| \le |s|.$$

Because J is continuously differentiable, we can choose a compact neighborhood of $\Lambda\times\{0\}\subset\mathbb{R}^m\times\mathbb{R}$ in which both $(DJ(u,s))$ and $(\partial_s J(u,s))$ are uniformly continuous. When s is sufficiently small, this neighborhood of $\Lambda\times\{0\}$ contains (u_i^s, s) for all i because $u_i^0\in\Lambda$ and u_i^s are i-uniformly continuously differentiable (from Theorem 1) and therefore are i-uniformly continuous. Also, $\dfrac{du_i^s}{ds}$ are i-uniformly continuous. Therefore, for all $\epsilon>0$, there exists $\delta>0$, such that for all $|\xi|<\delta$,

$$\|\gamma_i^{\xi}-\gamma_i^0\|<\epsilon\quad\forall i.$$

Therefore, for all $|s|<\delta$, $|\xi_i(s)|\le|s|\le\delta$ for all i, thus for all $n>0$,

$$\left\|\frac{1}{n}\sum_{i=1}^{n}\gamma_i^{\xi_i(s)}-\frac{1}{n}\sum_{i=1}^{n}\gamma_i^{0}\right\|\le\frac{1}{n}\sum_{i=1}^{n}\left\|\gamma_i^{\xi_i(s)}-\gamma_i^{0}\right\|<\epsilon\ .$$

thus,

$$\left\|\lim_{n\to\infty}\frac{1}{n}\sum_{i=1}^{n}\gamma_i^{\xi_i(s)}-\lim_{n\to\infty}\frac{1}{n}\sum_{i=1}^{n}\gamma_i^{0}\right\|\le\epsilon\ .$$

Therefore,

$$\left.\frac{d\langle J\rangle}{ds}\right|_{s=0} = \lim_{s\to 0}\lim_{n\to\infty}\frac{1}{n}\sum_{i=1}^{n}\gamma_i^{\xi_i(s)} = \lim_{n\to\infty}\frac{1}{n}\sum_{i=1}^{n}\gamma_i^{0}\ .$$

This competes the proof via the definition of γ_i^0 and $v_i^{\{\infty\}}$. ◻

With Theorem 5, we are one step away from the main theorem (Theorem LSS – the shadowing direction $v_i^{\{\infty\}}$ in Theorem 5 needs to be replaced by the solution $v_i^{\{n\}}$ to the least squares problems (1.3). The next section proves a bound of the distance between $v_i^{\{\infty\}}$ and $v_i^{\{n\}}$.

5. Computational approximation of shadowing direction. This section assumes all conditions of Theorem 1, and focus on when $s=0$. We denote u_i^0 by u_i in this section and the next section.

The main task of this section is providing a bound for

$$e_i^{\{n\}} = v_i^{\{n\}} - v_i^{\{\infty\}}\ ,\quad i=1,\ldots,n \tag{5.1}$$

where $v_i^{\{n\}}$ is the solution to the least squares problems

$$\min\frac{1}{2}\sum_{i=1}^{n}v_i^{\{n\}T}v_i^{\{n\}}\quad\text{s.t.}\quad v_{i+1}^{\{n\}}=(Df(u_i,0))\,v_i^{\{n\}}+(\partial_s f(u_i,0)),\quad i=1,\ldots,n-1. \tag{5.2}$$

This bound will enable us to show that the difference between $v_i^{\{n\}}$ and $v_i^{\{\infty\}}$ makes a vanishing difference in Equation (4.2) as $n\to\infty$.

Lemma 6. *$e_i^{\{n\}}$ as defined in Equation (5.1) satisfy*

$$e_{i+1}^{\{n\}} = (Df(u_i,0))\,e_i^{\{n\}}\ ,\quad i=1,\ldots,n-1 \tag{5.3}$$

In addition, their components in the stable and unstable directions, $e_i^{\{n\}+} \in V^+(u_i)$ *and* $e_i^{\{n\}-} \in V^-(u_i)$*, where* $e_i^{\{n\}+} + e_i^{\{n\}-} = e_i^{\{n\}}$*, satisfies*

$$e_{i+1}^{\{n\}+} = (Df(u_i,0))\, e_i^{\{n\}+}\ , \quad e_{i+1}^{\{n\}-} = (Df(u_i,0))\, e_i^{\{n\}-}\ , \quad i=1,\dots,n-1 \tag{5.4}$$

Proof. By definition, $u_{i+1}^s = f(u_i^s, s)$ for all s in a neighborhood of 0. By taking derivative to s on both sides, we obtain

$$v_{i+1}^{\{\infty\}} = (Df(u_i,0))v_i^{\{\infty\}} + (\partial_s f(u_i,0))$$

Subtracting this from the constraint in Equation (5.2), we obtain Equation (5.3).

By substituting $e_i^{\{n\}} = e_i^{\{n\}+} + e_i^{\{n\}-}$ into Equation (5.3), we obtain

$$\left(e_{i+1}^{\{n\}+} - (Df(u_i,0))\, e_i^{\{n\}+}\right) + \left(e_{i+1}^{\{n\}-} - (Df(u_i,0))\, e_i^{\{n\}-}\right) = 0$$

Because the spaces $V^+(u)$ and $V^-(u)$ are invariant (Equation (2.3)),

$$(Df(u_i,0))\, e_i^{\{n\}\pm} \in V^\pm(u_{i+1}), \quad \text{thus} \quad \left(e_{i+1}^{\{n\}\pm} - (Df(u_i,0))\, e_i^{\{n\}\pm}\right) \in V^\pm(u_{i+1})\ .$$

Because they sum to 0, both parentheses must be in $V^+(u_{i+1}) \cap V^-(u_{i+1}) = \{0\}$. This proves Equation (5.4). ∎

Lemma 6 indicates that for all ϵ^+ and ϵ^-,

$$v_i'^{\{n\}} = v_i^{\{n\}} + \epsilon^+ e_i^{\{n\}+} + \epsilon^- e_i^{\{n\}-} \tag{5.5}$$

satisfies the constraint in Problem (5.2), i.e.,

$$v_{i+1}'^{\{n\}} = (Df(u_i,0))\, v_i'^{\{n\}} + (\partial_s f(u_i,0)), \quad i=1,\dots,n-1\ .$$

Because $v_i^{\{n\}}$ is the solution to Problem (5.2), it must be true that

$$\sum_{i=1}^n v_i^{\{n\}T} v_i^{\{n\}} \le \sum_{i=1}^n v_i'^{\{n\}T} v_i'^{\{n\}} \qquad \text{for all } \epsilon^+ \text{ and } \epsilon^-\ .$$

By substituting the definition of v_i' in Equation (5.5), and use the first order optimality condition with respect to ϵ^+ and ϵ^- at $\epsilon^+ = \epsilon^- = 0$, we obtain

$$\sum_{i=1}^n v_i^{\{n\}T} e_i^{\{n\}+} = \sum_{i=1}^n v_i^{\{n\}T} e_i^{\{n\}-} = 0 \tag{5.6}$$

By substituting $v_i^{\{n\}} = v_i^{\{\infty\}} + e_i^{\{n\}} = v_i^{\{\infty\}} + e_i^{\{n\}+} + e_i^{\{n\}-}$ into Equation (5.6), we obtain

$$\begin{aligned}
&\sum_{i=1}^n (v_i^{\{\infty\}})^T e_i^{\{n\}+} + \sum_{i=1}^n (e_i^{\{n\}+})^T e_i^{\{n\}+} + \sum_{i=1}^n (e_i^{\{n\}-})^T e_i^{\{n\}+} = 0 \\
&\sum_{i=1}^n (v_i^{\{\infty\}})^T e_i^{\{n\}-} + \sum_{i=1}^n (e_i^{\{n\}+})^T e_i^{\{n\}-} + \sum_{i=1}^n (e_i^{\{n\}-})^T e_i^{\{n\}-} = 0
\end{aligned} \tag{5.7}$$

To transform Equation (5.7) into bounds on $e_i^{\{n\}+}$ and $e_i^{\{n\}-}$, we need the following lemma.

LEMMA 7. *The hyperbolic splitting of* $e_i^{\{n\}}$ *as defined in Equation (5.1) satisfies*

$$\|e_i^{\{n\}+}\| \le C\,\lambda^{n-i}\|e_n^{\{n\}+}\|\,, \quad \|e_i^{\{n\}-}\| \le C\,\lambda^{i}\|e_0^{\{n\}-}\|$$

Proof. This is a direct consequence of Equation (5.4) and the definition of V^+ and V^- in Equation (2.2). □

By combining the first equality in Equation (5.7) with Lemma 7 and using the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned}\|e_n^{\{n\}+}\|^2 &\le \sum_{i=1}^n (e_i^{\{n\}+})^T e_i^{\{n\}+} = -\sum_{i=1}^n (v_i^{\{\infty\}})^T e_i^{\{n\}+} - \sum_{i=1}^n (e_i^{\{n\}-})^T e_i^{\{n\}+} \\ &\le \sum_{i=1}^n \|v_i^{\{\infty\}}\|\|e_i^{\{n\}+}\| + \sum_{i=1}^n \|e_i^{\{n\}-}\|\|e_i^{\{n\}+}\| \\ &\le \sum_{i=1}^n C\,\lambda^{n-i}\|v_i^{\{\infty\}}\|\|e_n^{\{n\}+}\| + \sum_{i=1}^n C^2\lambda^n\|e_0^{\{n\}-}\|\|e_n^{\{n\}+}\|\end{aligned}$$

Therefore,

$$\|e_n^{\{n\}+}\| \le \frac{C}{1-\lambda}\left\|\mathbf{v}^{\{\infty\}}\right\|_{\mathcal{B}} + nC^2\lambda^n\|e_0^{\{n\}-}\|$$

where the $\mathcal{B}$ norm is as defined in Section 3, and is finite by Theorem 1. Similarly, By combining the second equality in Equation (5.7) with Lemma 7 and using the Cauchy-Schwarz inequality,

$$\|e_0^{\{n\}-}\| \le \frac{C}{1-\lambda}\left\|\mathbf{v}^{\{\infty\}}\right\|_{\mathcal{B}} + nC^2\lambda^n\|e_n^{\{n\}+}\|$$

When n is sufficiently large such that $nC^2\lambda^n < \frac{1}{3}$, we can substitute both inequalities into each other and obtain

$$\|e_n^{\{n\}+}\| \le \frac{2C}{1-\lambda}\left\|\mathbf{v}^{\{\infty\}}\right\|_{\mathcal{B}}\,, \quad \|e_n^{\{n\}-}\| \le \frac{2C}{1-\lambda}\left\|\mathbf{v}^{\{\infty\}}\right\|_{\mathcal{B}}\,, \tag{5.8}$$

This inequality leads to the following theorem that bounds the norm of $e_i^{\{n\}}$, the difference between the least squares solution $v_i^{\{n\}}$ and the shadowing direction.

THEOREM 8. *If* n *is sufficiently large such that* $3nC\lambda^n < 1$*, then* $e_i^{\{n\}}$ *as defined in Equation (5.1) satisfies*

$$\|e_i^{\{n\}}\| < \frac{2C^2}{1-\lambda}\left\|\mathbf{v}^{\{\infty\}}\right\|_{\mathcal{B}}(\lambda^i + \lambda^{n-i})\,, \quad i = 1,\ldots,n$$

Proof. From the hyperbolicity assumption (2.2) and Lemma 7,

$$\|e_i^{\{n\}}\| \le \|e_i^{\{n\}+}\| + \|e_i^{\{n\}-}\| \le C\,\lambda^{n-i}\|e_n^{\{n\}+}\| + C\,\lambda^i\|e_0^{\{n\}-}\|$$

The theorem is then obtained by substituting Equation (5.8) into $\|e_n^{\{n\}+}\|$ and $\|e_0^{\{n\}-}\|$ in the inequality above. □

This theorem shows that $v_i^{\{n\}}$ is a good approximation of the shadowing direction $v_i^{\{\infty\}}$ when n is large and $-\log\lambda \ll i \ll n + \log\lambda$. The next section shows that the approximation has a vanishing error in Equation (1.2) as $n \to \infty$. Combined with Theorem 5, we then prove a rigorous statement of Theorem LSS.

6. Convergence of least Squares sensitivity. This section uses the results of the previous sections to prove our main theorem.

THEOREM LSS. *For a C^1 map $f : \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}^m$, assume $f(\cdot, 0)$ is bijective and defines a compact global hyperbolic attractor Λ. For a C^1 map $J : \mathbb{R}^m \times \mathbb{R} \to \mathbb{R}$ whose infinite time average $\langle J \rangle$ as defined in Equation (4.1) is independent of the initial state $u_0 \in \mathbb{R}^m$. Then for all sequence $\{u_i, i \in \mathbb{Z}\} \subset \Lambda$ satisfying $u_{i+1} = f(u_i, 0)$,*

$$\left.\frac{d\langle J\rangle}{ds}\right|_{s=0} = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \Big((DJ(u_i,0))\, v_i^{\{n\}} + (\partial_s J(u_i,0)) \Big) \;, \tag{6.1}$$

where $v_i^{\{n\}} \in \mathbb{R}^m, i = 1, \ldots, n$ is the solution to the constrained least squares problem (1.3).

Proof. Because J is C^1 and Λ is compact, $(DJ(u_i, 0))$ is uniformly bounded, i.e., there exists A such that $\|(DJ(u_i, 0))\| < A$ for all i. Let $e_i^{\{n\}}$ be defined as in Equation (5.1), whose norm is bounded by Theorem 8, then for large enough n,

$$\begin{aligned}
&\left| \frac{1}{n} \sum_{i=1}^{n} \Big((DJ(u_i,0))\, v_i^{\{n\}} + (\partial_s J(u_i,0)) \Big) - \frac{1}{n} \sum_{i=1}^{n} \Big((DJ(u_i^0,0)) v_i^{\{\infty\}} + (\partial_s J(u_i^0,0)) \Big) \right| \\
&= \left| \frac{1}{n} \sum_{i=1}^{n} (DJ(u_i,0))\, e_i^{\{n\}} \right| \le \frac{1}{n} \sum_{i=1}^{n} \|(DJ(u_i,0))\|\, \|e_i^{\{n\}}\| \\
&< \frac{1}{n} \sum_{i=1}^{n} \frac{2A\,C^2}{1-\lambda} \left\| \mathbf{v}^{\{\infty\}} \right\|_{\mathcal{B}} (\lambda^i + \lambda^{n-i}) < \frac{1}{n} \frac{4A\,C^2}{(1-\lambda)^2} \left\| \mathbf{v}^{\{\infty\}} \right\|_{\mathcal{B}} \xrightarrow{n\to\infty} 0
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \Big((DJ(u_i,0))\, v_i^{\{n\}} + (\partial_s J(u_i,0)) \Big) \\
&= \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} \Big((DJ(u_i,0)) v_i^{\{\infty\}} + (\partial_s J(u_i,0)) \Big) = \left.\frac{d\langle J\rangle}{ds}\right|_{s=0}
\end{aligned}$$

by Theorem 5. ∎

7. The least squares sensitivity algorithm. A practicible algorithm based on Theorem LSS is the following.

1. Choose large enough n_0 and n, and an arbitrary starting point $u_{-n_0} \in \mathbb{R}^m$.
2. Compute $u_{i+1} = f(u_i, s), i = -n_0, \ldots, 0, 1, \ldots, n$.
   For large enough n_0, $u_1, \ldots, u_n$ are approximately on the global attractor Λ.
3. Solve the system of linear equations

$$\begin{cases} v_{i+1} = (Df(u_i,s))\, v_i + (\partial_s f(u_i,s)), & i = 1, \ldots, n-1 \\ w_{i-\frac12} = (Df(u_i,s))^T w_{i+\frac12} + v_i \;, & i = 1, \ldots, n \\ w_{\frac12} = w_{n+\frac12} = 0 & \end{cases}$$

   which is the first order optimality condition of the constrained least squares problem (1.3), and gives its unique solution $v_1, \ldots, v_n$. Note that a linear relation between $w_{i-\frac12}, w_{i+\frac12}$ and $w_{i+\frac32}$ can be obtained by substituting the second equation into the first one. A block tridiagonal solver can then be used to solve the system.

4. Compute the desired derivative by

$$\frac{d\langle J\rangle}{ds} \approx \frac{1}{n}\sum_{i=1}^{n}\left(\left(DJ(u_i,0)\right)v_i + \left(\partial_s J(u_i,0)\right)\right) \,.$$

Theorem LSS shows that the computed derivative is accurate for large n. This algorithm is implemented in the Python code **lssmap**, available at https://github.com/qiqi/lssmap

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